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# 2,5,7-Trimethyl-3-phenylsulfonyl-1-benzofuran

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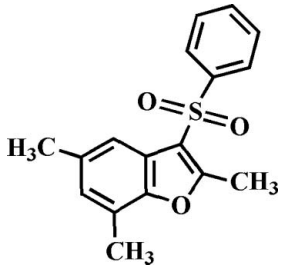
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.037; $wR$ factor = 0.104; data-to-parameter ratio = 16.6.

The title compound, $C_{17}H_{16}O_3S$, was prepared by the oxidation of 2,5,7-trimethyl-3-phenylsulfanyl-1-benzofuran with 3-chloroperoxybenzoic acid. The phenyl ring exhibits a dihedral angle of 81.16 (4)° with the plane of the benzofuran fragment. The crystal structure is stabilized by $\pi$–$\pi$ interactions between the furan and benzene rings of neighbouring molecules [centroid–centroid distance = 3.874 (2) Å] and by C—H$\cdots\pi$ interactions between a phenyl H atom of the phenylsulfonyl substituent and the furan ring of adjacent molecules. In addition, the crystal structure exhibits intra- and intermolecular C—H$\cdots$O interactions.

## Related literature

For the crystal structures of similar substituted benzofuran compounds, see: Choi *et al.* (2007*a*,*b*).




## Experimental

### Crystal data

$C_{17}H_{16}O_3S$
$M_r$ = 300.36
Monoclinic, $P2_1/n$
$a$ = 9.2468 (7) Å
$b$ = 8.4238 (7) Å
$c$ = 18.963 (2) Å
$\beta$ = 91.535 (2)°
$V$ = 1476.6 (2) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.23 mm$^{-1}$
$T$ = 173 (2) K
0.40 × 0.40 × 0.10 mm

### Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
8704 measured reflections
3212 independent reflections
2544 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.041

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.104
$S$ = 1.03
3212 reflections
193 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.38 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C12—H12$\cdots Cg1^{i}$ | 0.95 | 2.81 | 3.747 (3) | 169 |
| C16—H16$C\cdots$O3$^{ii}$ | 0.98 | 2.48 | 3.403 (2) | 158 |
| C17—H17$A\cdots$O2 | 0.98 | 2.42 | 3.135 (3) | 129 |

Symmetry codes: (i) $-x+1, -y+2, -z$; (ii) $-x+2, -y+1, -z$. $Cg1$ is the centroid of the O1/C8/C1/C2/C7 furan ring.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2106).

## References

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Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
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# supporting information

*Acta Cryst.* (2008). E**64**, o794 [doi:10.1107/S1600536808008477]

## 2,5,7-Trimethyl-3-phenylsulfonyl-1-benzofuran

**Hong Dae Choi, Pil Ja Seo, Byeng Wha Son and Uk Lee**

### S1. Comment

This work is related to earlier communications on the synthesis and structure of substituted benzofuran analogues, *viz*. 2,5-dimethyl-3-methylsulfinyl-1-benzofuran (Choi *et al.*, 2007*a*) and 2,5-dimethyl-3-phenylsulfinyl-1-benzofuran (Choi *et al.*, 2007*b*). Herein we report the molecular and crystal structure of the title compound, 2,5,7-trimethyl-3-phenylsulfonyl-1-benzofuran (Fig. 1).

The benzofuran unit is almost planar, with a mean deviation of 0.009 Å from the least-squares plane defined by the nine constituent atoms. The phenyl ring (C9—C14) is almost perpendicular to the plane of the benzofuran ring system [81.16 (4) °] and is tilted slightly towards it. The crystal packing (Fig. 2) is stabilized by aromatic $\pi$—$\pi$ stacking interactions between the furan and the benzene rings from neighbouring molecules. The *Cg*1···*Cg*2$^{ii}$ distance is 3.874 (2)Å (*Cg*1 and *Cg*2 are the centroids of the O1/C8/C1/C2/C7 furan ring and the C2—C7 benzene ring, respectively, symmetry code as in Fig. 2). The molecular packing is further stabilized by C—H···$\pi$ interactions between a phenyl H atom of the phenylsulfonyl substituent and the furan ring of the benzofuran unit, with a C12—H12···*Cg*$^{i}$ separation of 2.81 Å (Fig. 2 and Table 1; *Cg*1 is the centroid of the O1/C8/C1/C2/C7 furan ring, symmetry code as in Fig. 2). Additionally, intra- and intermolecular C—H···O interactions in the structure were observed (Fig. 2 and Table 1; symmetry code as in Fig. 2).

### S2. Experimental

3-Chloroperoxybenzoic acid (77%, 471 mg, 2.1 mmol) was added in small portions to a stirred solution of 2,5,7-trimethyl-3-phenylsulfanyl-1-benzofuran (268 mg, 1.0 mmol) in dichloromethane (30 ml) at 273 K. After being stirred for 4 h at room temperature, the mixture was washed with saturated sodium bicarbonate solution and the organic layer was separated, dried over magnesium sulfate, filtered and concentrated in vacuum. The residue was purified by column chromatography (hexane-ethyl acetate, 2:1 *v*/*v*) to afford the title compound as a colorless solid [yield 81%, m.p. 399–400 K; $R_f$ = 0.61 (hexane-ethyl acetate, 2:1 *v*/*v*)]. Single crystals suitable for X-ray diffraction were prepared by evaporation of a solution of the title compound in benzene at room temperature. Spectroscopic analysis: $^1$H NMR ($CDCl_3$, 400 MHz) $\delta$ 2.41 (s, 6H), 2.80 (s, 3H), 6.92 (s, 1H), 7.47–7.52 (m, 4H), 8.01 (d, J = 7.68 Hz, 2H); EI—MS 300 [$M^+$].

### S3. Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 Å for aromatic H atoms, 0.99 Å for methylene H atoms and 0.98 Å for methyl H atoms, respectively, and with $U_{iso}$(H) = 1.2Ueq(C) for aromatic and methylene, $U_{iso}$(H) =1.5Ueq(C) for H atoms for methyl H atoms.

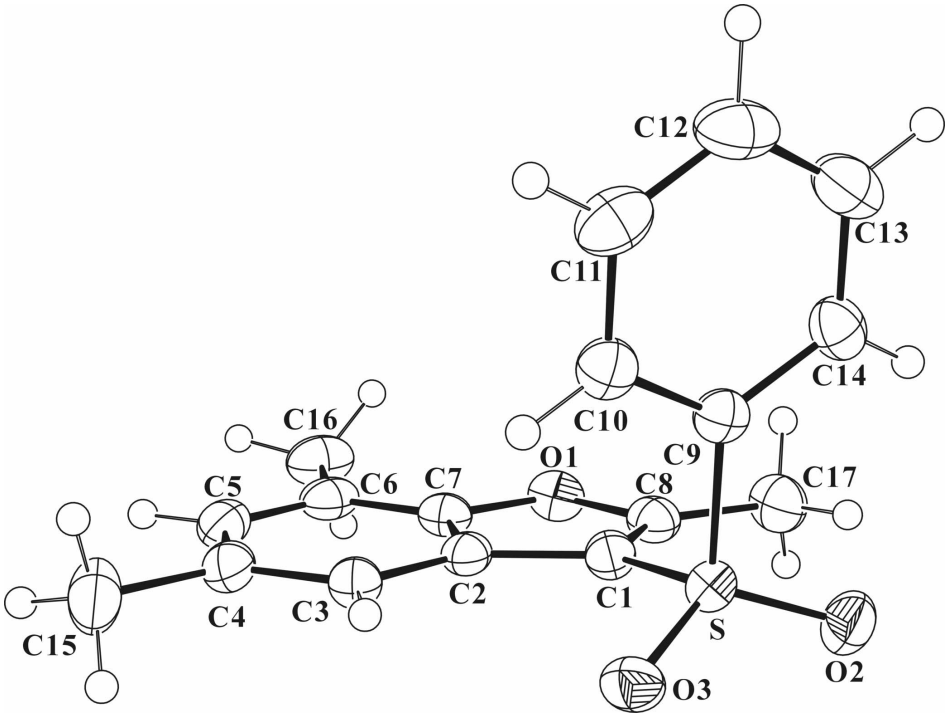


**Figure 1**

The molecular structure of the title compound, showing displacement ellipsoides drawn at the 50% probability level.

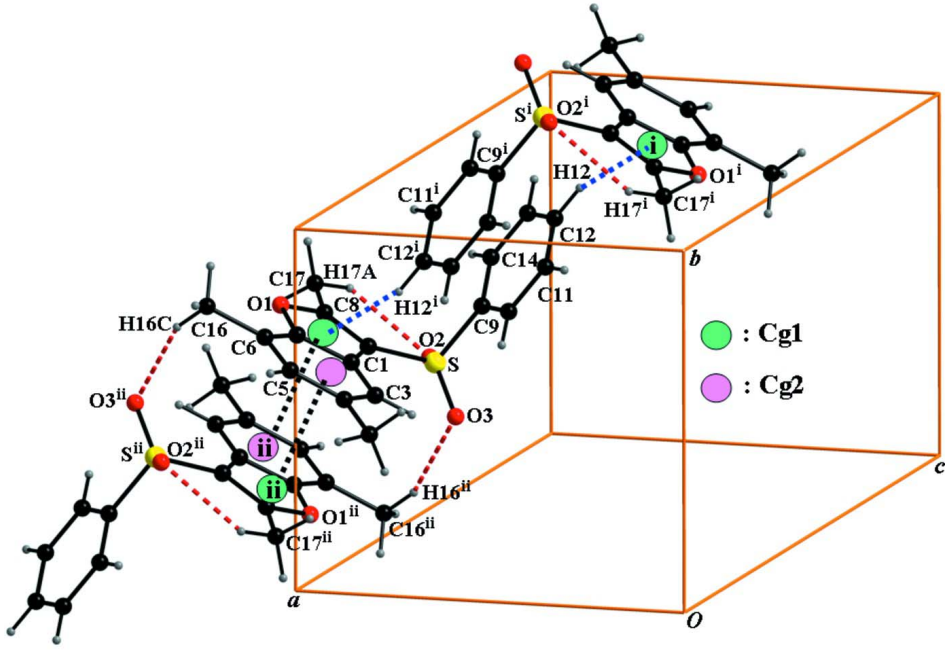


**Figure 2**

*π*—*π*, C—H···*π* and C—H···O interactions (dotted lines) in the title compound. *Cg* denotes the ring centroid. [Symmetry code: (i) -*x* + 1, -*y* + 2, -*z*; (ii) -*x* + 2, -*y* + 1, -*z*.]

## 2,5,7-Trimethyl-3-phenylsulfonyl-1-benzofuran

*Crystal data*

$C_{17}H_{16}O_3S$
$M_r = 300.36$
Monoclinic, $P2_1/n$
Hall symbol: -p 2yn
$a = 9.2468$ (7) Å
$b = 8.4238$ (7) Å
$c = 18.963$ (2) Å
$\beta = 91.535$ (2)°
$V = 1476.6$ (2) Å$^3$
$Z = 4$
$F(000) = 632$
$D_x = 1.351$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4291 reflections
$\theta = 2.5$–$28.3°$
$\mu = 0.23$ mm$^{-1}$
$T = 173$ K
Block, colorless
0.40 × 0.40 × 0.10 mm

*Data collection*

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.0 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
8704 measured reflections
3212 independent reflections
2544 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.5°$
$h = -11 \rightarrow 11$
$k = -7 \rightarrow 10$
$l = -24 \rightarrow 23$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.104$
$S = 1.04$
3212 reflections
193 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0467P)^2 + 0.6422P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å$^{-3}$
$\Delta\rho_{min} = -0.38$ e Å$^{-3}$

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted $R$-factor $wR$ and goodness of fit $S$ are based on $F^2$, conventional $R$-factors $R$ are based on $F$, with $F$ set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating $R$-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. $R$-factors based on $F^2$ are statistically about twice as large as those based on $F$, and $R$- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S | 0.71396 (5) | 0.59940 (5) | 0.11202 (2) | 0.02746 (13) |
| O1 | 1.04792 (13) | 0.77976 (15) | 0.01610 (7) | 0.0331 (3) |
| O2 | 0.77401 (15) | 0.57958 (16) | 0.18201 (6) | 0.0386 (3) |
| O3 | 0.63915 (14) | 0.46890 (14) | 0.07823 (7) | 0.0346 (3) |
| C1 | 0.84920 (18) | 0.6601 (2) | 0.05599 (9) | 0.0270 (4) |

| | | | | |
|---|---|---|---|---|
| C2 | 0.84265 (18) | 0.6499 (2) | −0.02041 (9) | 0.0260 (4) |
| C3 | 0.74772 (19) | 0.5861 (2) | −0.07118 (9) | 0.0290 (4) |
| H3 | 0.6625 | 0.5321 | −0.0579 | 0.035* |
| C4 | 0.7809 (2) | 0.6035 (2) | −0.14184 (9) | 0.0330 (4) |
| C5 | 0.9071 (2) | 0.6844 (2) | −0.16049 (10) | 0.0346 (4) |
| H5 | 0.9266 | 0.6957 | −0.2092 | 0.042* |
| C6 | 1.00483 (19) | 0.7488 (2) | −0.11156 (10) | 0.0328 (4) |
| C7 | 0.96763 (19) | 0.7270 (2) | −0.04190 (9) | 0.0291 (4) |
| C8 | 0.97377 (19) | 0.7376 (2) | 0.07465 (9) | 0.0304 (4) |
| C9 | 0.59363 (18) | 0.7624 (2) | 0.11293 (9) | 0.0263 (4) |
| C10 | 0.48964 (19) | 0.7768 (2) | 0.05910 (9) | 0.0318 (4) |
| H10 | 0.4830 | 0.7005 | 0.0223 | 0.038* |
| C11 | 0.3956 (2) | 0.9051 (2) | 0.06032 (11) | 0.0402 (5) |
| H11 | 0.3232 | 0.9165 | 0.0242 | 0.048* |
| C12 | 0.4063 (2) | 1.0159 (2) | 0.11345 (12) | 0.0450 (5) |
| H12 | 0.3416 | 1.1035 | 0.1137 | 0.054* |
| C13 | 0.5111 (2) | 1.0004 (2) | 0.16670 (11) | 0.0428 (5) |
| H13 | 0.5180 | 1.0776 | 0.2032 | 0.051* |
| C14 | 0.6058 (2) | 0.8729 (2) | 0.16692 (10) | 0.0329 (4) |
| H14 | 0.6777 | 0.8615 | 0.2033 | 0.040* |
| C15 | 0.6791 (2) | 0.5378 (3) | −0.19827 (10) | 0.0461 (5) |
| H15A | 0.6497 | 0.4301 | −0.1853 | 0.069* |
| H15B | 0.7282 | 0.5348 | −0.2434 | 0.069* |
| H15C | 0.5934 | 0.6058 | −0.2027 | 0.069* |
| C16 | 1.1407 (2) | 0.8345 (2) | −0.13129 (12) | 0.0438 (5) |
| H16A | 1.1486 | 0.9339 | −0.1046 | 0.066* |
| H16B | 1.1370 | 0.8581 | −0.1819 | 0.066* |
| H16C | 1.2249 | 0.7675 | −0.1202 | 0.066* |
| C17 | 1.0431 (2) | 0.7849 (2) | 0.14286 (10) | 0.0398 (5) |
| H17A | 0.9787 | 0.7586 | 0.1814 | 0.060* |
| H17B | 1.0614 | 0.8994 | 0.1427 | 0.060* |
| H17C | 1.1348 | 0.7278 | 0.1495 | 0.060* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S | 0.0317 (2) | 0.0259 (2) | 0.0248 (2) | 0.00101 (17) | 0.00055 (16) | 0.00232 (17) |
| O1 | 0.0278 (6) | 0.0313 (7) | 0.0401 (7) | −0.0011 (5) | 0.0010 (5) | −0.0019 (6) |
| O2 | 0.0440 (8) | 0.0429 (8) | 0.0287 (7) | 0.0047 (6) | −0.0027 (6) | 0.0058 (6) |
| O3 | 0.0403 (7) | 0.0252 (6) | 0.0383 (7) | −0.0040 (5) | 0.0022 (6) | −0.0008 (5) |
| C1 | 0.0264 (8) | 0.0274 (9) | 0.0273 (8) | 0.0029 (7) | −0.0003 (6) | −0.0001 (7) |
| C2 | 0.0276 (8) | 0.0229 (8) | 0.0276 (8) | 0.0051 (7) | 0.0019 (6) | 0.0015 (7) |
| C3 | 0.0301 (9) | 0.0280 (9) | 0.0289 (9) | 0.0026 (7) | 0.0005 (7) | 0.0000 (7) |
| C4 | 0.0383 (10) | 0.0317 (9) | 0.0289 (9) | 0.0091 (8) | −0.0003 (7) | 0.0010 (8) |
| C5 | 0.0430 (10) | 0.0332 (10) | 0.0281 (9) | 0.0124 (8) | 0.0082 (8) | 0.0045 (8) |
| C6 | 0.0334 (10) | 0.0260 (9) | 0.0395 (10) | 0.0081 (7) | 0.0098 (8) | 0.0050 (8) |
| C7 | 0.0287 (8) | 0.0238 (8) | 0.0348 (9) | 0.0043 (7) | 0.0007 (7) | −0.0003 (7) |
| C8 | 0.0294 (9) | 0.0274 (9) | 0.0343 (9) | 0.0047 (7) | −0.0008 (7) | −0.0013 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C9 | 0.0253 (8) | 0.0252 (8) | 0.0286 (8) | −0.0030 (7) | 0.0045 (7) | 0.0023 (7) |
| C10 | 0.0320 (9) | 0.0308 (9) | 0.0324 (9) | −0.0035 (7) | 0.0006 (7) | 0.0012 (8) |
| C11 | 0.0303 (10) | 0.0424 (11) | 0.0480 (12) | 0.0021 (8) | 0.0011 (8) | 0.0113 (9) |
| C12 | 0.0404 (11) | 0.0350 (11) | 0.0605 (13) | 0.0097 (9) | 0.0177 (10) | 0.0049 (10) |
| C13 | 0.0488 (12) | 0.0338 (10) | 0.0465 (12) | 0.0003 (9) | 0.0147 (9) | −0.0076 (9) |
| C14 | 0.0339 (9) | 0.0345 (10) | 0.0307 (9) | −0.0040 (8) | 0.0066 (7) | −0.0033 (8) |
| C15 | 0.0492 (12) | 0.0601 (14) | 0.0285 (10) | 0.0059 (11) | −0.0055 (8) | −0.0026 (9) |
| C16 | 0.0401 (11) | 0.0361 (11) | 0.0561 (13) | 0.0031 (9) | 0.0161 (10) | 0.0097 (9) |
| C17 | 0.0359 (10) | 0.0416 (11) | 0.0413 (11) | 0.0006 (9) | −0.0096 (8) | −0.0055 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S—O2 | 1.4346 (13) | C9—C10 | 1.389 (2) |
| S—O3 | 1.4401 (13) | C10—C11 | 1.388 (3) |
| S—C1 | 1.7394 (17) | C10—H10 | 0.9500 |
| S—C9 | 1.7674 (17) | C11—C12 | 1.375 (3) |
| O1—C8 | 1.367 (2) | C11—H11 | 0.9500 |
| O1—C7 | 1.384 (2) | C12—C13 | 1.387 (3) |
| C1—C8 | 1.363 (2) | C12—H12 | 0.9500 |
| C1—C2 | 1.451 (2) | C13—C14 | 1.386 (3) |
| C2—C3 | 1.393 (2) | C13—H13 | 0.9500 |
| C2—C7 | 1.396 (2) | C14—H14 | 0.9500 |
| C3—C4 | 1.390 (2) | C15—H15A | 0.9800 |
| C3—H3 | 0.9500 | C15—H15B | 0.9800 |
| C4—C5 | 1.405 (3) | C15—H15C | 0.9800 |
| C4—C15 | 1.511 (3) | C16—H16A | 0.9800 |
| C5—C6 | 1.388 (3) | C16—H16B | 0.9800 |
| C5—H5 | 0.9500 | C16—H16C | 0.9800 |
| C6—C7 | 1.386 (2) | C17—H17A | 0.9800 |
| C6—C16 | 1.505 (3) | C17—H17B | 0.9800 |
| C8—C17 | 1.483 (2) | C17—H17C | 0.9800 |
| C9—C14 | 1.386 (2) | | |
| | | | |
| O2—S—O3 | 119.48 (8) | C11—C10—C9 | 118.54 (17) |
| O2—S—C1 | 109.43 (8) | C11—C10—H10 | 120.7 |
| O3—S—C1 | 107.29 (8) | C9—C10—H10 | 120.7 |
| O2—S—C9 | 108.03 (8) | C12—C11—C10 | 120.53 (19) |
| O3—S—C9 | 107.59 (8) | C12—C11—H11 | 119.7 |
| C1—S—C9 | 103.94 (8) | C10—C11—H11 | 119.7 |
| C8—O1—C7 | 106.96 (13) | C11—C12—C13 | 120.35 (19) |
| C8—C1—C2 | 107.46 (15) | C11—C12—H12 | 119.8 |
| C8—C1—S | 126.78 (14) | C13—C12—H12 | 119.8 |
| C2—C1—S | 125.53 (13) | C14—C13—C12 | 120.26 (19) |
| C3—C2—C7 | 119.27 (16) | C14—C13—H13 | 119.9 |
| C3—C2—C1 | 136.18 (16) | C12—C13—H13 | 119.9 |
| C7—C2—C1 | 104.55 (15) | C13—C14—C9 | 118.66 (18) |
| C4—C3—C2 | 118.31 (17) | C13—C14—H14 | 120.7 |
| C4—C3—H3 | 120.8 | C9—C14—H14 | 120.7 |

| | | | |
|---|---|---|---|
| C2—C3—H3 | 120.8 | C4—C15—H15A | 109.5 |
| C3—C4—C5 | 119.98 (17) | C4—C15—H15B | 109.5 |
| C3—C4—C15 | 119.65 (18) | H15A—C15—H15B | 109.5 |
| C5—C4—C15 | 120.36 (17) | C4—C15—H15C | 109.5 |
| C6—C5—C4 | 123.47 (17) | H15A—C15—H15C | 109.5 |
| C6—C5—H5 | 118.3 | H15B—C15—H15C | 109.5 |
| C4—C5—H5 | 118.3 | C6—C16—H16A | 109.5 |
| C7—C6—C5 | 114.32 (17) | C6—C16—H16B | 109.5 |
| C7—C6—C16 | 122.04 (18) | H16A—C16—H16B | 109.5 |
| C5—C6—C16 | 123.64 (17) | C6—C16—H16C | 109.5 |
| O1—C7—C6 | 124.99 (16) | H16A—C16—H16C | 109.5 |
| O1—C7—C2 | 110.38 (15) | H16B—C16—H16C | 109.5 |
| C6—C7—C2 | 124.63 (17) | C8—C17—H17A | 109.5 |
| C1—C8—O1 | 110.64 (15) | C8—C17—H17B | 109.5 |
| C1—C8—C17 | 134.26 (17) | H17A—C17—H17B | 109.5 |
| O1—C8—C17 | 115.10 (15) | C8—C17—H17C | 109.5 |
| C14—C9—C10 | 121.66 (17) | H17A—C17—H17C | 109.5 |
| C14—C9—S | 119.35 (14) | H17B—C17—H17C | 109.5 |
| C10—C9—S | 118.98 (13) | | |

| | | | |
|---|---|---|---|
| O2—S—C1—C8 | −24.52 (19) | C3—C2—C7—O1 | −179.24 (14) |
| O3—S—C1—C8 | −155.54 (16) | C1—C2—C7—O1 | 0.79 (18) |
| C9—S—C1—C8 | 90.68 (17) | C3—C2—C7—C6 | 1.4 (3) |
| O2—S—C1—C2 | 161.63 (14) | C1—C2—C7—C6 | −178.60 (16) |
| O3—S—C1—C2 | 30.61 (17) | C2—C1—C8—O1 | 0.6 (2) |
| C9—S—C1—C2 | −83.18 (16) | S—C1—C8—O1 | −174.20 (12) |
| C8—C1—C2—C3 | 179.23 (19) | C2—C1—C8—C17 | −179.81 (19) |
| S—C1—C2—C3 | −5.9 (3) | S—C1—C8—C17 | 5.4 (3) |
| C8—C1—C2—C7 | −0.81 (19) | C7—O1—C8—C1 | −0.07 (19) |
| S—C1—C2—C7 | 174.03 (13) | C7—O1—C8—C17 | −179.78 (15) |
| C7—C2—C3—C4 | −0.7 (2) | O2—S—C9—C14 | 20.07 (16) |
| C1—C2—C3—C4 | 179.30 (18) | O3—S—C9—C14 | 150.32 (14) |
| C2—C3—C4—C5 | −0.3 (3) | C1—S—C9—C14 | −96.11 (15) |
| C2—C3—C4—C15 | −179.10 (17) | O2—S—C9—C10 | −160.35 (13) |
| C3—C4—C5—C6 | 0.8 (3) | O3—S—C9—C10 | −30.10 (15) |
| C15—C4—C5—C6 | 179.52 (17) | C1—S—C9—C10 | 83.47 (15) |
| C4—C5—C6—C7 | −0.1 (3) | C14—C9—C10—C11 | −0.5 (3) |
| C4—C5—C6—C16 | 179.55 (17) | S—C9—C10—C11 | 179.95 (13) |
| C8—O1—C7—C6 | 178.91 (16) | C9—C10—C11—C12 | 0.5 (3) |
| C8—O1—C7—C2 | −0.48 (18) | C10—C11—C12—C13 | −0.2 (3) |
| C5—C6—C7—O1 | 179.76 (15) | C11—C12—C13—C14 | −0.1 (3) |
| C16—C6—C7—O1 | 0.1 (3) | C12—C13—C14—C9 | 0.2 (3) |
| C5—C6—C7—C2 | −0.9 (3) | C10—C9—C14—C13 | 0.1 (3) |
| C16—C6—C7—C2 | 179.37 (16) | S—C9—C14—C13 | 179.70 (14) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C12—H12···*Cg*1$^{i}$ | 0.95 | 2.81 | 3.747 (3) | 169 |
| C16—H16*C*···O3$^{ii}$ | 0.98 | 2.48 | 3.403 (2) | 158 |
| C17—H17*A*···O2 | 0.98 | 2.42 | 3.135 (3) | 129 |

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*; (ii) −*x*+2, −*y*+1, −*z*.